

Sunday, June 10, 2001

1:00 pm 7:00 pm	Registration/Check-In Reception	Quail Ridge Inn Resort
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Monday, June 11, 2001

8:20 Opening Remarks G. L. Kellogg

8:30 Welcome

Session 1 Bio-Surface Interfaces I Chair: Paul Weiss

8:40 H. G. Craighead (Invited Talk)
School of Applied and Engineering Physics, Cornell University, Ithaca, NY
“Manipulation and Analysis of Molecules in Nanofluidic Systems”

9:20 Hyun I. Kim and J. E. Houston
Sandia National Laboratories, Albuquerque, NM
“‘Interphase’ Liquid Structure and Interfacial Forces”

9:40 Bruce C. Bunker¹, D. Huber¹, J. Kushmerick¹, C. Matzke¹, J. F. Stoddard², J. Cao², J. O. Jeppesen², and J. Perkins²
¹*Sandia National Laboratories, Albuquerque, NM*
²*University of California at Los Angeles, Los Angeles, CA*
“Controlled Switching of Surface Chemistry Using Tethered Molecular Machines”

10:00 Break

Session 2 Bio-Surface Interfaces II Chair: Terry Michalske

10:30 George D. Bachand¹ and Carlo D. Montemagno²
¹*Sandia National Laboratories, Albuquerque, NM*
²*Department of Biological and Environmental Engineering, Cornell University, Ithaca, NY*
“Biotechnology at the Molecular Scale: The Use of Biological Motors as Actuators in Nano-Electro-Mechanical Systems”

10:50 P. S. Weiss¹, P. A. Lewis¹, R. K. Smith¹, B. A. Mantooth¹, L. A. Bumm¹, K. F. Kelly¹, S. M. Reed², R. S. Clegg², and J. E. Hutchison²
¹*Department of Chemistry, Pennsylvania State University, University Park, PA*
²*Department of Chemistry, University of Oregon, Eugene, OR*
“Manipulating Phase Behavior by Varying Buried Functionality in Monolayers: STM Investigation of Alkanethiols and Amide-Containing Alkanethiols”

11:10 K. F. Kelly¹, Z. J. Donhauser¹, B. A. Mantooth¹, J. D. Monell¹, L. A. Bumm¹, J. J. Stapleton¹, D. L. Allara¹, P. S. Weiss¹, D. W. Price, Jr.², and J. M. Tour²
¹*Department of Chemistry, The Pennsylvania State University, University Park, PA*
²*Department of Chemistry, Rice University, Houston, TX*
“Conductance Switching in Single Molecules Through Conformational Changes”

11:30 V.A. Samuilov, Y.-S. Seo, D. Gersappe, J. Sokolov, M. Rafailovich
Department of Materials Science, SUNY at Stony Brook, Stony Brook, NY
“Mesoscopic Patterning and Electrical Transport of Long DNA Molecules on Liquid-Solid Interfaces”

11:50 J. G. Tobin¹, K.R. Wilson¹, and R. J. Saykally²
¹*Lawrence Livermore National Laboratory, Livermore, CA*
²*Department of Chemistry, University of California, Berkeley, CA*
“X-Ray Absorption Spectroscopy of Liquid and Gaseous Water”

12:10 Lunch

Session 3 Bio-Sensors and Adatom Studies

Chair: Jack Houston

- 1:30 D. Y. Petrovykh^{1,2}, M. J. Yang², and L. J. Whitman²
¹Physics Department, University of Maryland, College Park, MD
²Naval Research Laboratory, Washington, DC
“Surface Passivation and Functionalization of InAs”
- 1:50 R. J. Colton¹, M. M. Miller¹, M. A. Piani², J. C. Rife¹, P. E. Sheehan¹, C. R. Tamanaha³, and L. J. Whitman¹
¹Naval Research Laboratory, Washington, DC
²Nova Research, Inc., Alexandria, VA
³Geo-Centers, Inc., Fort Washington, MD
“Sensing Biomolecules with Magnetics: The BARC Biosensor”
- 2:10 B.S. Swartzentruber¹, M. L. Grant², J. B. Hannon², and N. C. Bartelt³
¹Sandia National Laboratories, Albuquerque, NM
²Carnegie Mellon University, Pittsburgh, PA
³Sandia National Laboratories, Livermore, CA
“Vacancy-Mediated Diffusion of Pd on Cu(001) Measured with Atom-Tracking STM”
- 2:30 Peter J. Feibelman¹ and Thomas Michely²
¹Sandia National Laboratories, Albuquerque, NM
²I. Physikalisches Institut, RWTH-Aachen, Aachen, Germany
“Pt-dimer Dissociation on Pt(111)”
- 2:50 E. Lundgren¹, M. Borg¹, J. N. Andersen¹, R. Nyholm¹, X. Torelles², C. Konvicka³, M. Schmid³, and P. Varga³
¹Department of Synchrotron Radiation Research, Institute of Physics, Lund University, Lund, Sweden
²Institut de Ciencia de Materials de Barcelona (C.S.I.C), Bellaterra, Barcelona, Spain
³Institut für Allgemeine Physik, Technische Universität Wien, Wien, Austria
“The Surface Induced Valence Transition in Sm(0001): A Direct View”
- 3:10 Break

Session 4 Computational Surface Dynamics

Chair: Art Voter

- 3:30 K. Thüermer¹, J.E. Reutt-Robey², Ellen D. Williams^{1,3}, M. Uwaha⁴
¹Department of Physics, University of Maryland, College Park, MD
²Department of Chemistry, University of Maryland, College Park, MD
³Institute for Physical Science and Technology, University of Maryland, College Park, MD
⁴Department of Physics, Nagoya University, Nagoya, Japan
“A Step Dynamics Picture of Crystal Shape Relaxations”
- 3:50 J. A. Sprague, F. Montalenti, and A. F. Voter
Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM
“Heteroepitaxial Growth by Temperature Accelerated Molecular Dynamics Simulations: Cu Films and Cu/Ag Superlattices on Ag (100)”
- 4:10 F. Montalenti and A. F. Voter
Los Alamos National Laboratory, Los Alamos, NM
“Atomistic Simulation of Crystal Growth at Experimental Deposition Fluxes: Ag/Ag(100)”
- 4:30 Kenneth Haug
Department of Chemistry, Lafayette College, Easton, PA
“Comparison of Computational Kinetics Methods Applied to the Effects of Hydrogen on the Epitaxial Growth of Ni Surfaces”

6:00 Picnic (Pool and Patio Area)

Tuesday, June 12, 2001

Session 5 The Nottingham Competition
Chair: Brian Swartzentruber

- 8:40 C. N. Borca and P. A. Dowben
Brace Laboratory and the Center of Material Research and Analysis, University of Nebraska, Lincoln, NE
“Evidence for Temperature Dependent Moment Ordering in Ferromagnetic NiMnSb(100) Thin Films”
- 9:00 H. Ohldag and J. Stöhr
Stanford Synchrotron Radiation Laboratory, Stanford University, Stanford, CA
“Chemical and Magnetic Characterization of Buried Antiferromagnet-Ferromagnet Interfaces Using Polarization Dependent Photoemission Electron Spectromicroscopy”
- 9:20 T. E. Kidd¹ and T.-C. Chiang²
¹*Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL*
²*Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, IL*
“APRES Investigation of a Charge Density Wave at the Sn/Ge(111) $3 \times 3R30^0$ Surface”
- 9:40 Dustin A. Hite and Phillip T. Sprunger
Department of Physics and Astronomy and the J. Bennett Johnston, Sr. Center for Advanced Microstructures and Devices Louisiana State University, Baton Rouge, LA
“Electronic Structure of Surface-Confined Alloys in Bulk-Immiscible Systems”
- 10:00 Break
- 10:30 J. Ledieu and R. McGrath
Surface Science Research Centre, The University of Liverpool, Liverpool, United Kingdom
“The Five-Fold Surface of Al₇₀Pd₂₁Mn₉: Tiling and C₆₀ Adsorption”
- 10:50 B. L. M. Hendriksen and J. W. M. Frenken
Kamerlingh Onnes Laboratorium, Universiteit Leiden, Leiden, The Netherlands
“A Model Catalyst in Action”
- 11:10 G. Thayer
Physics Department, University of California at Davis, Davis, CA
Sandia National Laboratories, Livermore, CA
“Linking Stress to Surface Structure Using STM”
- 11:30 Thomas P. Pearl and S. J. Sibener
The James Franck Institute and Department of Chemistry, The University of Chicago, Chicago, IL
“Oxygen Driven Reconstruction Dynamics and Mechanistic Details of a Stepped Metallic Surface Measured by Time-Lapse Scanning Tunneling Microscopy”
- 11:50 Mellita Caragiu and R. D. Diehl
Pennsylvania State University, University Park, PA
“Low-Energy Electron Diffraction Studies of Rare Gases Adsorbed on Metal Surfaces”
- 12:10 Lunch

Session 6 Surface Theory
Chair: Norm Bartelt

- 1:30 Ann E. Mattsson
Sandia National Laboratories, Albuquerque, NM
“Energy Functionals for Surface Systems”
- 1:50 Matthias Scheffler (**Invited Talk**)
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany
“Get Real! The Importance of Complexity for Understanding and for Predictive Calculations of the Properties and Function of Surfaces”

- 2:30 Alexander Bogicevic¹ and Dwight R. Jennison²
¹ *Scientific Research Laboratories, Ford Motor Company, Dearborn, MI*
² *Sandia National Laboratories, Albuquerque, NM*
 “Metal Adsorption and Island Nucleation on Ionic Metal-Oxide Terraces”
- 2:50 Frank Grosse^{1,2}, William Barvosa-Carter¹, Jennifer J. Zinck¹, Mark F. Gyure¹
¹ *HRL Laboratories LLC, Malibu, CA*
² *Department of Mathematics, University of California, Los Angeles, CA*
 “Atomistic Modeling of III/V Semiconductors: Thermodynamic Equilibrium and Growth Kinetics”
- 3:10 Break

Session 7 Surface Atomic Structure and Phase Transitions
Chair: Thomas Mattsson

- 3:30 J. B. Hannon, J. Tersoff, and R. M. Tromp
IBM Research Division, T. J. Watson Research Center, Yorktown Heights, NY
 “Surface Stress and the Morphology of Si(111) Near Tc”
- 3:50 M. Kammler¹, Horn von Högen¹, N. Voss², M. Tringides², A. Menzel³, and E. H. Conrad³
¹ *Fachbereich Physik, Universität Essen, Essen, Germany*
² *Ames Laboratory, Iowa State University, Ames, IA*
³ *School of Physics, Georgia Institute of Technology, Atlanta, GA*
 “Si(100) Step Dynamics: A Temporal Low Energy Diffraction Study”
- 4:10 K. H. Wu, M. Ono, K. Nakayama, T. Nagao and T. Sakurai
Institute for Material Research, Tohoku University, Sendai, Japan
 “Two-state Adsorption and Self-Aligned Clustering of Na on the Si(111)-7x7 Surface”
- 4:30 W. Barvosa-Carter^{1,2}, R. S. Ross¹, C. Ratsch^{1,2}, F. Grosse^{1,2}, J. H. G. Owen^{1,2}, M. Gyure¹ and J. J. Zinck¹
¹ *HRL Laboratories LLC, Malibu, CA*
² *Department of Mathematics, University of California, Los Angeles, CA*
 “(2 x4)-Reconstructed InAs(001) Surfaces at Low and High As₂ Pressure in an MBE Environment Studied Using STM and DFT”
- 4:50 Richard Plass¹, Norm C. Bartelt², and G. L. Kellogg¹
¹ *Sandia National Laboratories, Albuquerque, NM*
² *Sandia National Laboratories, Livermore, CA*
 “Pb on Cu(111): Self-Assembled Surface Domain Structures”

7:00 Conference Banquet (Dining Room)

Wednesday, June 13, 2001

Session 8 Oxide and Nitride Surfaces

Chair: Dwight Jennison

- 8:40 J. A. Kelber
Department of Chemistry, University of North Texas, Denton, TX
“Metallization of Silicate Surfaces: Unusual Oxide Surfaces for Microelectronics Interconnect Applications”
- 9:00 A. Arya and Emily A. Carter
Department of Chemistry and Biochemistry, University of California at Los Angeles, Los Angeles, CA
“First-Principles Studies of Electronic and Structural Properties of TiC, ZrC and BN Surfaces”
- 9:20 J. J. Joyce, A. J. Arko, T. Durakiewicz, D. P. Moore and L. Morales
Los Alamos National Laboratory, Los Alamos, NM
“Plutonium Surface and Interface Development: Cleaning, Oxides and Hydrogen Dosing”
- 9:40 Haiqiang Yang¹, Hamad Al-Brithen¹, Arthur R. Smith¹, J. A. Borchers², R. L. Cappelletti², and M. D. Vaudin²
¹*Department of Physics and Astronomy, Ohio University, Athens, OH*
²*National Institute of Standards and Technology, Gaithersburg, MD*
“Surface and Bulk Structure of Manganese Nitride Films Grown by Molecular Beam Epitaxy”
- 10:00 Break

Session 9 Surface Epitaxy

Chair: John Joyce

- 10:30 T.-C. Shen
Department of Physics, Utah State University, Logan, UT
“Low Temperature Silicon Epitaxy on Si(100) Monohydride Surfaces”
- 10:50 A. Mans, A. R. H. F. Ettema and H. H. Weitering
Electronic Materials Group, Department of Applied Physics, Delft University of Technology, Delft, The Netherlands
“Multilayer Relaxations in Magic Thin Films”
- 11:10 Q. Z. Xue and T. Sakurai
Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
“Molecular Beam Epitaxy-Scanning Tunneling Microscopy of Wurtzite GaN Thin Films”
- 11:30 C. L. Chen¹, J. Shen¹ and Y. Lin¹, J. C. Jiang², E. I. Meletis², F. W. Van Keuls³ and F. A. Miranda³
¹*The Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX*
²*Mechanical Engineering Department, Louisiana State University, Baton Rouge, LA*
³*NASA Glenn Research Center, Communications Technology Division, Cleveland, OH*
“Epitaxial Growth and Interface Structures of Ferroelectric Thin Films”
- 12:10 Lunch

Session 10 Electronic Structure and Surface Chemistry

Chair: Neal Shinn

- 1:30 T. Durakiewicz¹, J. J. Joyce¹, A. J. Arko¹, D. P. Moore¹, L. A. Morales¹, J. L. Sarrao¹, S. Halas², J. Sikora³, and W. Krolopp³
¹*Los Alamos National Laboratory, Los Alamos, NM*
²*Maria Curie-Sklodowska University, Institute of Physics, Lublin, Poland*
³*Technical University of Lublin, Lublin, Poland*
“Electronic Work Function of Actinides”
- 1:50 D. L. Jaeger, T. Tyler, V. V. Zhirnov, A. Kvit, J. J. Hren
North Carolina State University, Department of Material Science and Engineering, Raleigh, NC
“Dynamic Effects of Local Electric Fields on the Evolution of Nanodiamond Coatings”

- 2:30 J. N. Russell, Jr.¹, D. Fitzgerald², D. Doren², J. S. Hovis³, R. J. Hamers³, G. T. Wang⁴, S.F. Bent⁴, M. P. D'Evelyn⁵, and J. E. Butler¹
¹Chemistry Division, Naval Research Laboratory, Washington, DC
²Department of Chemistry, University of Delaware, Newark, DE
³Department of Chemistry, University of Wisconsin, Madison, WI
⁴Department of Chemical Engineering, Stanford University, Stanford, CA
⁵Corporate Research and Development, General Electric, Schenectady, NY
 “Influence of Electronic Screening on the Infrared Spectrum of Hydrogen on Diamond (100)”
- 2:50 Maritoni Litorja and Steven A. Buntin
 National Institute of Standards and Technology, Gaithersburg, MD
 “The Oxidation of Deuterium-, Ethylene- and Acetylene-Terminated Si(100) by Atomic Oxygen”
- 3:10 Break

Session 11 Device Fabrication and Characterization

Chair: Toshio Sakurai

- 3:30 V. W. Ballarotto, K. Siegrist, R. J. Phaneuf and E. D. Williams
 Laboratory for Physical Sciences and Department of Physics University of Maryland, College Park, MD
 “Dopant-Induced Contrast of Si Devices in PEEM”
- 3:50 T. Yamada¹, N. Takano², K. Yamada², S. Yoshitomi², T. Inoue² and T. Osaka²
¹Kagami Memorial Laboratory for Materials Science and Technology, Waseda University, Tokyo, Japan
²School of Science and Engineering, Waseda University, Tokyo, Japan
 “Possibilities of Electron Beam Nanometer-scale Fabrication of Si(111) Using Alkyl Monolayers”
- 4:10 Y. Fujikawa, J. T. Sadowski, K. F. Kelly, K. S. Nakayama and T. Sakurai
 Institute for Materials Research, Tohoku University, Sendai, Japan
 “Comparison of Adsorption and Etching of F₂ and C₆₀F_x on Si(111)-7x7”
- 4:30 Rikard A. Wind¹, Martin J. Murtagh², Fang Mei², Yu Wang¹, Stephen L. Sass², and Melissa A. Hines¹
¹Department of Chemistry, Cornell University, Ithaca, NY
²Department of Materials Science and Engineering, Cornell University, Ithaca, NY
 “Towards Nanofabrication at the Molecular Scale: Controlled Etching of Dislocations in Bonded Silicon”
- 4:50 V. N. Enteev, M. V. Moiseenko, N. A. Slusarenko, S. L. Legusha, and E. Ya. Glushko
 Pedagogical University, Krivoy Rog, Ukraine
 “Charging Effects in Quantum Fragments of Molecular Electronics Devices”